Comment on “Optimal Reaction Time for Surface-Mediated Diffusion”

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In recent letter [Phys. Rev. Lett **105**, 150606 (2010)], the surface-mediated diffusion problem is theoretically discussed, and interesting results have been obtained. However, for more general cases, the ansatz of solutions of the diffusion equation, which is the starting point of their analysis, might not be appropriate. In this comment, suggested ansatz and corresponding methods will be presented.

PACS numbers: 05.40.Fb

For the surface-mediated process studied in [1], in which a molecule diffuses in a spherical confining domain of radius R and alternates phases of boundary diffusion (with diffusion coefficient D_1) and phases of bulk diffusion (with diffusion coefficient D_2), the mean first-passage (MFPT) at the target, i.e., parts of the boundary $r = R$: $\theta \in [0, \epsilon] \cup [2\pi - \epsilon, 2\pi]$, satisfies the following equation

$$t_1''(\theta) - \sigma\lambda t_1(\theta) = -\sigma[1 + \lambda t_2(R - a, \theta)], \qquad (1)$$

for $\theta \in [\epsilon, 2\pi - \epsilon]$. Where $t_1(\theta)$ is the MFPT starting from the boundary defined by angle θ, λ is dissociation rate from the boundary to bulk, a is the distance that the molecule is assumed to be ejected once it is dissociated from the boundary, and $\sigma = R^2/D_1$. $t_2(r, \theta)$ is the MFPT staring from point (r, θ), which satisfies

$$D_2(\partial_r^2 + \partial_r/r + \partial_\theta^2/r^2)t_2(r, \theta) = -1. \qquad (2)$$

The boundary conditions of Eqs. (1) (2) are $t_2(R, \theta) = t_1(\theta)$ and $t_1(\theta) = 0$ for $\theta \in [0, \epsilon] \cup [2\pi - \epsilon, 2\pi]$ respectively.

In [1] and also in their more recent work [2], the following ansatz is assumed to be the solutions of Eq. (2)

$$t_2(r, \theta) = \alpha_0 - \frac{r^2}{4D_2} + \sum_{n=1}^{\infty} \alpha_n r^n \cos(n\theta), \qquad (3)$$

where α_n are constants to be determined. Based on this ansatz, interesting results have been drawn in [1]. However, mathematically, it can be easily shown that a more general form of the solutions of Eq. (2) is

$$\begin{aligned} t_2(r, \theta) =& \alpha_0(1 + \mu \ln r)(1 + \gamma\theta) - \frac{r^2}{4D_2} \\ &+ \sum_{n=\pm 1}^{\pm\infty} r^n[\alpha_n \cos(n\theta) + \beta_n \sin(n\theta)], \end{aligned} \qquad (4)$$

where $\alpha_n, \beta_n, \mu, \gamma$ are constants to be determined. For most of the physical or biophysical processes, it is reasonable to assume that $t_2(0, \theta) < \infty$. Therefore, the general form (4) can be simplified to

$$\begin{aligned} t_2(r, \theta) =& \alpha_0(1 + \gamma\theta) - \frac{r^2}{4D_2} \\ &+ \sum_{n=1}^{\infty} r^n[\alpha_n \cos(n\theta) + \beta_n \sin(n\theta)], \end{aligned} \qquad (5)$$

In a general aspect, the ansatz (5) might be more appropriate than ansata (3).

To obtain the MFPT $\langle t_1 \rangle$, in [1], Eq. (1) is solved approximately by perturbative expansion, and then another approximate method is developed in [2]. Here, I will suggest another method. For the general form (5) of $t_2(r, \theta)$, the solution $t_1(\theta)$ of Eq. (1) can be obtained explicitly (we assume $a \neq R$ and $\lambda \neq 0$),

$$\begin{aligned} t_1(\theta) =& c_1 e^{\sqrt{\sigma\lambda\theta}} + c_2 e^{-\sqrt{\sigma\lambda\theta}} \\ &+ \alpha_0(1 + \gamma\theta) - \frac{(R-a)^2}{4D_2} + \frac{1}{\lambda} \\ &+ \sum_{n=1}^{\infty} \frac{(R-a)^n}{n^2/\sigma\lambda + 1}[\alpha_n \cos(n\theta) + \beta_n \sin(n\theta)], \end{aligned} \qquad (6)$$

where constants c_1, c_2 are determined by boundary conditions $t_1(\epsilon) = t_1(2\pi - \epsilon) = 0$, and $\alpha_0, \alpha_n, \beta_n$ can be obtained by $t_2(R, \theta) = t_1(\theta)$ and Eqs. (5) and (6).

If $a = R$ or $\lambda = 0$, then Eq. (1) is reduced to $t_1''(\theta) = -\sigma$. Its solution is

$$t_1(\theta) = \sigma(2\pi - \epsilon - \theta)(\theta - \epsilon)/2. \qquad (7)$$

Then the MFPT $\langle t_1 \rangle$ can be easily obtained by integral $\int_\epsilon^{2\pi-\epsilon} t_1 d\theta$.

It should be pointed out that the above discussion is only valid for λ is constant. In real physical process, λ will decrease with a, and $\lambda \to \infty$ when $a \to 0$. Therefore the formulation (7) is only an instructive approximation.

[1] O. Bénichou, D. Grebenkov, P. Levitz, C. Loverdo, and R. Voituriez, *Phys. Rev. Lett.* **105**, 150606 (2010).
[2] O. Bénichou, D. Grebenkov, P. Levitz, C. Loverdo, and R. Voituriez, *J. Stat. Phys.* **142**, 657 (2011).